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Non-Leptonic Kaon Decays and the Chiral Regime of the Strong Interaction

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We present a status report on our project to investigate the origins of the $\Delta I = 1/2$ rule in $K \to \pi\pi$ decays using lattice simulations of Quantum Chromodynamics (QCD). In particular, we seek to clarify the rôle of the charm quark, which has long been suspected to be important for the enhancement of the $\Delta I = 1/2$ transition amplitude. Among the main ingredients of our calculation is the use of fermionic discretisations which preserve chiral symmetry at non-zero lattice spacing. Furthermore, we keep an active charm quark at all stages of the calculation. Finally, we connect $K \to \pi\pi$ amplitudes to the computationally simpler $K \to \pi$ transitions by matching QCD to Chiral Perturbation Theory in the so-called ϵ-regime. This necessitates performing simulations very close to the massless limit. We report on the associated numerical difficulties and how they can be solved via an exact treatment of a number of low-lying eigenmodes of the discretised Dirac operator.

1 Introduction

K-mesons are quark-antiquark bound states in which one light quark flavour (up or down) is paired with a "strange" flavour. Since the weak interaction does not conserve strangeness, kaons exhibit many different decay modes[1], as well as mixing phenomena, such as oscillations between a neutral K-meson, K^0, and its antiparticle, $\bar{K}^0$. The decay and mixing patterns of kaons are important sources of information for our understanding of fundamental symmetries and their violations. In the Standard Model CP symmetry, which transforms particles into antiparticles, is not conserved. The strength of CP violation in weak decays is determined by the elements of the so-called Cabibbo-Kobayashi-Maskawa (CKM) matrix, and a lot of experimental and theoretical activity is currently spent to pin down their values with high accuracy.

However, many efforts of gaining quantitative insight into weak processes involving kaons are hampered by effects of the strong interaction: kaon decays cannot simply be treated at the level of weak transitions between their fundamental constituents, i.e. the quarks, as the latter are subjected to effects of the strong interaction as well. In principle, these effects can be computed in Quantum Chromodynamics (QCD), the gauge theory of the strong interaction. However, since the strong coupling constant is not small at typical hadronic mass scales, perturbative QCD is totally inadequate for providing a quantitative description in this regime. Non-leptonic kaon decays are perhaps one of the most striking examples for this failure: if a neutral kaon, having isospin 1/2, decays into a pair of pions, the latter can either have isospin $I = 0$ or 2. The corresponding transition amplitudes are then given by the amplitudes A_0 and A_2 (up to a phase factor). The experimentally observed decay rates yield an unexpectedly large ratio of

$$A_0/A_2 \approx 22.1, \tag{1}$$

which implies that the decay in which isospin changes by 1/2 is favoured over the $\Delta I = 3/2$ transition by a large margin, and this observation is usually called the $\Delta I = 1/2$ rule. By contrast, theoretical calculations based purely on perturbative QCD can only provide a crude estimate for A_0/A_2 which turns out to be smaller by a full order of magnitude! It remains a major challenge to explain the experimentally observed enhancement in the framework of QCD.

The formulation of QCD on a discrete space-time lattice is designed specifically for a non-perturbative treatment. However, decays like $K \to \pi\pi$ are notoriously difficult to address directly in lattice QCD[2,3]. Here we follow the path of obtaining information on $K \to \pi\pi$ decays via the theoretically much simpler $K \to \pi$ transition[9]. The connection to the amplitudes A_0 and A_2 is then provided by matching results from lattice simulations of QCD to an effective low-energy description of the strong interaction, called Chiral Perturbation Theory[4].

The aim of our project is to understand the mechanism which is responsible for the $\Delta I = 1/2$ rule. In particular we seek to clarify whether the observed large enhancement in A_0 over A_2 has a single origin or if it is the result of an accumulation of several moderately large effects. To this end we specifically concentrate on the rôle of the charm quark and the fact that – owing to its large mass of around 1.3 GeV – it decouples from typical low-energy QCD scales of a few hundred MeV. Unlike all previous lattice studies we use a formulation in which the charm quark is "active" in the sense that it is not integrated out from the theory. We first determine the amplitudes A_0 and A_2 for the unphysical situation where the charm is degenerate with the light quark, $m_c = m_u = m_d = m_s$. In a second step we envisage monitoring the amplitudes for heavier charm, i.e. $m_c > m_u = m_d = m_s$. In this note we concentrate on the mass-degenerate case.

In order to keep this note accessible to a wider readership, we skip most technical details and instead refer to our previous papers [5–8].

2 Matching QCD to Chiral Perturbation Theory

Chiral Perturbation Theory (ChPT) is an effective theory of the strong interaction: its fundamental fields are not the quarks and gluons of the QCD but rather the pseudo-Goldstone bosons associated with the spontaneous breaking of chiral symmetry, i.e. the pions, kaons and η-mesons. ChPT is parameterised in terms of empirical coupling constants ("low-energy constants" – LECs) which incorporate the short-distance effects of the strong interaction, but are not calculable in ChPT. They must be computed from the underlying theory of QCD, e.g. by matching predictions of ChPT to simulation data of lattice QCD, but are usually only determined phenomenologically using experimental data.

Since we are interested in investigating the rôle of the charm quark in $K \to \pi\pi$ we first consider the mass-degenerate case $m_c = m_u = m_d = m_s$. At leading order in ChPT the amplitudes A_0 and A_2 are then related to LECs g_1^+ and g_1^- via

$$\frac{A_0}{A_2} = \frac{1}{\sqrt{2}} \left(\frac{1}{2} + \frac{3}{2} \frac{g_1^-}{g_1^+} \right). \tag{2}$$

At lowest order the effective interaction which describes $K \to \pi\pi$ transitions in terms of Goldstone fields is given by [a]

$$\mathcal{H}_{\rm w}^{\rm ChPT} = 2\sqrt{2} G_{\rm F} (V_{us})^* V_{ud} \left\{ g_1^+ [\widehat{\mathcal{O}}_1^+] + g_1^- [\widehat{\mathcal{O}}_1^-] \right\}, \tag{3}$$

where the operators $\widehat{\mathcal{O}}_1^\pm$ mediate transitions in which strangeness changes by one unit. The expression in eq. (3) is the effective low-energy transcription of the corresponding Hamiltonian in QCD, i.e.

$$\mathcal{H}_{\rm w} = \sqrt{2} G_{\rm F} (V_{us})^* V_{ud} \left\{ k_1^+ \mathcal{Q}_1^+ + k_1^- \mathcal{Q}_1^- \right\}, \tag{4}$$

and the operators $\mathcal{Q}_1^\pm$ are expressed in terms of quark fields according to

$$\mathcal{Q}_1^\pm = \Big\{ (\overline{s}\gamma_\mu P_- u)(\overline{u}\gamma_\mu P_- d) \pm (\overline{s}\gamma_\mu P_- d)(\overline{u}\gamma_\mu P_- u) \Big\} - (u \to c). \tag{5}$$

The Wilson coefficients $k_1^\pm$ in the above expression absorb short-distance effects and can be computed reliably in perturbation theory. With these definitions, one can formulate a matching condition between ChPT and QCD, which allows to express the unknown LECs $g_1^\pm$ in terms of *correlation functions* that are evaluated in lattice simulations, as well as some additional known factors:

$$\frac{g_1^-}{g_1^+} H(x_0, y_0) = \frac{k_1^-}{k_1^+} \cdot \frac{\widehat{Z}^-}{\widehat{Z}^+} \cdot \frac{C_1^-(x_0, y_0)}{C_1^+(x_0, y_0)}. \tag{6}$$

Here, $C_1^\pm(x_0, y_0)$ denote three-point correlation functions of the operators $\mathcal{Q}_1^\pm$ and left-handed axial currents which are used as interpolating operators for the kaon and pion at Euclidean times x_0 and y_0, respectively [5]:

$$C_1^\pm(x_0, y_0) = \sum_{\vec{x}, \vec{y}} \left\langle (\overline{d}\gamma_0 P_- u)(x)\, \mathcal{Q}_1^\pm(0)\, (\overline{u}\gamma_0 P_- s)(y) \right\rangle, \quad P_- = \tfrac{1}{2}(1 - \gamma_5). \tag{7}$$

The factors $\widehat{Z}^\pm$ are inserted to account for the proper renormalisation of the operators $\mathcal{Q}_1^\pm$. [10,8] Finally, the chiral correction factor $H(x_0, y_0)$ is the ChPT counterpart of the ratio of correlation functions C_1^-/C_1^+, and can be computed in ChPT [5].

In its original formulation[4] ChPT is an expansion in quark masses and momenta about the massless limit. In this case the chiral correction factor H can only be computed at leading order, since otherwise $\mathcal{H}_{\rm w}^{\rm ChPT}$ must be supplemented with additional interaction terms, whose coefficients are not known, so that predictivity is lost. From a conceptual

[a] Here $G_{\rm F}$ is the Fermi constant, and V_{us}, V_{ud} are CKM matrix elements.

point of view, an alternative kinematical region of ChPT is of particular interest: the so-called ϵ-regime[11] is defined by formulating the theory in a finite volume and for arbitrarily small quark masses:

$$m\Sigma V \lesssim 1. \tag{8}$$

Here m denotes the quark mass, Σ the chiral condensate, and V is the space-time volume. In this situation, the chiral counting rules change in such a way that at next-to-leading order no further terms in addition to those of eq. (3) must be taken into account. Therefore, if one succeeds in performing the difficult numerical task of simulating close to the massless limit, the LECs $g_1^{\pm}$ can be extracted with H determined beyond leading order. Furthermore, long chiral extrapolations, which were the main weakness of previous lattice studies, can be avoided.

3 Lattice Set-Up and Simulations

In all our simulations chiral symmetry is preserved at non-zero lattice spacing. A sufficient condition for this to be the case is the Ginsparg-Wilson relation, i.e.

$$\gamma_5 D + D\gamma_5 = aD\gamma_5 D, \tag{9}$$

where a is the lattice spacing, and D the discretised Dirac operator[12,13]. A particular solution to this relation is defined by the Neuberger-Dirac operator[14], which we have used in our simulations. Preserving chiral symmetry has two key advantages for our project: first, it allows for a clean matching between ChPT and QCD, since the underlying assumption in standard ChPT is that chiral symmetry is only softly broken by the quark masses. Second, chiral symmetry protects the operators $\mathcal{Q}_1^{\pm}$ against mixing with lower-dimensional operators[10]. Thus, the complicated non-perturbative subtraction procedures outlined in[2] can be completely avoided.

The disadvantage of using Ginsparg-Wilson fermions is their large computational cost. A particular definition of the massless Neuberger-Dirac operator is given by

$$D_{\mathrm{N}} = \frac{1}{a}\left\{1 - \frac{A}{\sqrt{A^{\dagger}A}}\right\}, \qquad A = 1 - aD_{\mathrm{w}}, \tag{10}$$

where D_{w} is the usual Wilson-Dirac operator. The inverse square root in eq. (10) must be approximated by a polynomial in the matrix A. The degree of this polynomial, which is typically of O(50-100), then serves as an estimate how much more expensive one single application of D_{N} is in comparison to $A = 1 - aD_{\mathrm{w}}$. Although efficient numerical techniques have been developed, especially for the ϵ-regime[15], practically all current simulations employing the Neuberger-Dirac operator are performed in the quenched approximation. Since our primary aim is not focused on a high-precision calculation but rather on explaining a large non-perturbative effect, the quenched approximation appears appropriate for this task.

During our first calculations of the correlation functions $C_1^{\pm}$ in the ϵ-regime, we observed extremely large statistical fluctuations, whose origin could be traced back to the spectrum of the Neuberger-Dirac operator. To illustrate the point it is instructive to consider the spectral representation of the quark propagator, which is just the inverse of the

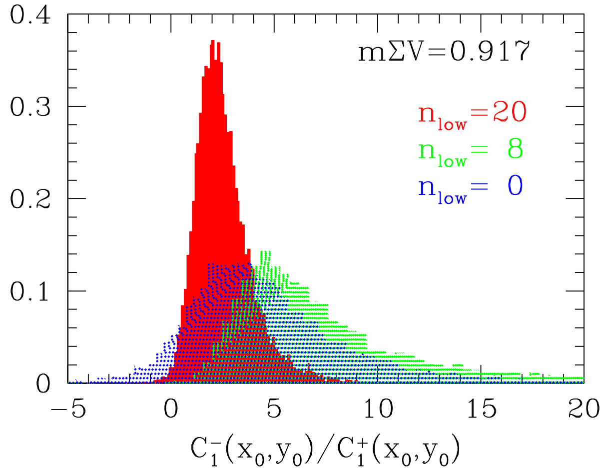

Figure 1. Bootstrap distributions of C_1^-/C_1^+ for $x_0/a = 5, y_0/a = 15$ at $\beta = 5.8$ on $8^3 \cdot 20$.

Dirac operator. It reads

$$S(x,y) = \frac{1}{V}\sum_i \frac{\eta_i(x) \otimes \eta_i(y)^\dagger}{\lambda_i + m}, \tag{11}$$

where $\eta_i(x)$ is an eigenvector of the Neuberger-Dirac operator with eigenvalue λ_i. If the quark mass is of the same size as the smallest eigenvalue or even smaller, it no longer provides an infrared cutoff on the spectrum. It is then possible that the contribution of a few low-lying modes are amplified by the denominator in eq. (11), so that they completely dominate in $S(x,y)$. Moreover, low modes $\eta_i(x)$ whose local magnitude at the point x exceeds the average magnitude by far can also make a dominant contribution to the propagator, if their weight in the spectral sum is enhanced by means of a small eigenvalue. As a result, the Monte Carlo history of correlation functions may exhibit a number of isolated “spikes”, where individual gauge configurations produce values which differ by several orders of magnitude from the ensemble average. A reliable error estimate is then not possible, and the signal is virtually lost.

It turned out that the bulk of the extreme fluctuations can be cured by separating off a number of low-lying modes and treating their contributions exactly[16,17]. This technique was first tested successfully in the simpler case of two-point correlation functions[17] and subsequently extended to the three-point functions $C_1^\pm$. The effectiveness of this procedure is shown in Fig. 1. Here we plot bootstrap distributions of the ratio C_1^-/C_1^+ for a particular choice of timeslices x_0, y_0. The plot clearly shows increasingly peaked distributions as the number of low modes that are treated exactly is increased. We emphasise that without low-mode averaging it is practically impossible to obtain a meaningful signal in the ϵ-regime.

Our main results were obtained on a lattice of size $16^3 \cdot 32$ at a bare gauge coupling g_0 corresponding to $\beta \equiv 6/g_0^2 = 5.8485$. At this value the lattice spacing in physical units is $a \approx 0.12\,\text{fm}$. We computed as many as 20 lowest-lying modes of the Neuberger-Dirac operator, using the techniques described in[15]. Furthermore, the gauge configurations were sorted according to their topological index $|\nu|$, which counts the number of exact zero

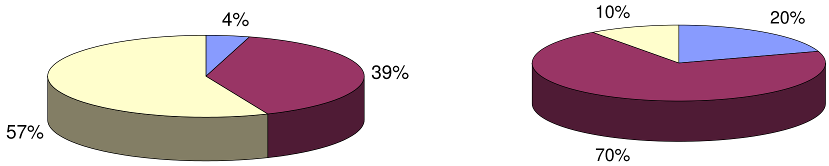

Figure 2. Left: the fraction of CPU time required for computing low modes of D_{w} (blue), low modes of D_{N} (purple) and correlation functions (white); Right: CPU time for the correlators (i.e. 57% of the total) divided up further into percentages spent on inversions (blue), low-mode averaging (purple) and propagator traces (white).

modes of D_{N}. In addition to computing $C_1^{\pm}$ for two quark masses which lie in the ϵ-regime, we also considered four heavier masses. This allows us to investigate the systematics of our calculation, by comparing our results computed directly near the massless limit with those obtained from chiral extrapolations from those heavier masses.

Our code is written in standard C, and was originally developed and optimised for PC clusters. Thus, we made extensive use of SSE/SSE2 inline assembly statements, which on an IBM facility like JUMP had to be switched off during compilation. The code allows for communication in two of the four space-time directions, implemented via the Message Passing Interface (MPI) library. On JUMP we typically used 32 processors for our $16^3 \cdot 32$ lattice. The typical compute speed for one application of the Wilson-Dirac operator was about 1 GFlops per processor. It is interesting to compare this with the performance on a PC cluster: on the cluster at DESY Hamburg, which uses Intel Xeon 1.7 GHz CPUs along with Myrinet 2000 as the communication interconnect we achieved 950 MFlops with 32-bit arithmetics, and around 500 MFlops in 64-bit precision.

On JUMP the calculation of three-point functions for two quark masses in the ϵ-regime with 20 low-lying eigenvectors used in the low-mode averaging procedure takes on average 23 hours of CPU time for a single configuration. A detailed comparison of CPU times for the various parts of the code is shown in Fig. 2. It is interesting to note that almost 90% of the total CPU time is spent on manipulations involving the low-lying modes of the Neuberger-Dirac operator. We also wish to point out that the CPU time required to determine the index ν and the lowest non-zero eigenmodes can fluctuate quite strongly. Small values of $|\nu|$ are more frequently associated with very small eigenvalues, and in this case our algorithm needs more iterations to distinguish reliably between a mode with a small but non-zero eigenvalue and an exact zero mode. On our $16^3 \cdot 32$ lattice the maximum time required to compute the low modes could be as much as 18 hours (that is, twice the average time required for this step), which is close to the limit of the `n_long` queue. Larger lattices can therefore only be considered on JUMP if we parallelise the code in more than two space-time directions.

4 Results and Outlook

We shall now present our preliminary results for three-point correlation functions computed for a light, degenerate charm quark. In each topological sector characterised by $|\nu|$

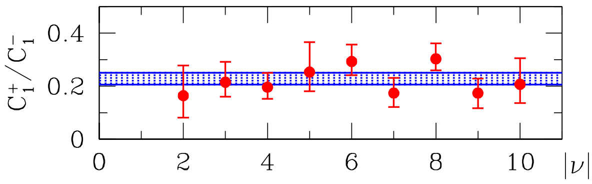

Figure 3. Results for the fitted ratio C_1^+/C_1^- in each topological sector. The weighted average is represented by the blue band.

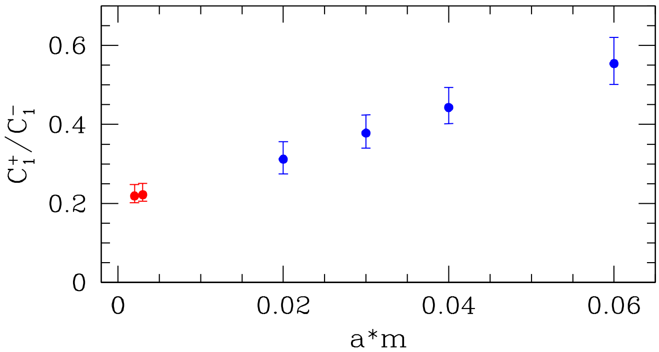

Figure 4. Quark mass dependence of the ratio C_1^+/C_1^-. The four points coloured in blue lie outside the ϵ-regime.

we fitted the correlation function $C_1^{\pm}(x_0, y_0)$ to a constant in the intervals $x_0/a \in [9, 12]$ and $y_0/a \in [20, 23]$. In Fig. 3 we plot the ratio of the fitted correlators, C_1^+/C_1^-, for each sector $|\nu|$. The formulae of ChPT in the ϵ-regime at NLO predict that this ratio should not show any dependence on $|\nu|$, and indeed our data are practically constant within errors. We therefore performed a weighted average over topological sectors, which has the added advantage that those sectors which suffer most from statistical fluctuations caused by the low-lying modes barely contribute to the final result.

The dependence of C_1^+/C_1^- on the quark mass is depicted in Fig. 4. Here we also show the four data points at heavier masses, i.e. outside the ϵ-regime. The data exhibit a smooth mass dependence, but one should be aware that over the whole mass range the data points are subjected to non-uniform chiral corrections, which must be taken into account before results for the combination of LECs g_1^-/g_1^+ can be quoted. A detailed investigation of these corrections is currently underway. Hence, we refrain from quoting an estimate for g_1^-/g_1^+ and instead refer the reader to a forthcoming paper[18].

Here we simply state that our preliminary analysis indicates that for a light, degenerate charm quark the ratio of amplitudes A_0/A_2 is significantly larger than the value derived in early order-of-magnitude theoretical estimates, but that it still falls way short of the experimental result. Our future work will focus on corroborating the current findings, but more importantly we shall consider larger charm quark masses to study their effects in relation to the $\Delta I = 1/2$ rule directly. First test runs are currently being performed.

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